

Ambiguities on the Hamiltonian formulation of the free falling particle with quadratic dissipation

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Abstract

For a free falling particle moving in a media which has quadratic velocity force effect on the particle, two equivalent constants of motion, with units of energy, two Lagrangians, and two Hamiltonians are deduced. These quantities describe the dynamics of the same classical system. However, their quantization and the associated statistical mechanics (for an ensemble of particles) describe two completely different quantum and statistical systems. This is shown at first order in the dissipative parameter.

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1 Introduction

It is well known that the Lagrangian (therefore the Hamiltonian) formulation for some systems of more than one dimension may not exists (Douglas 1941). Fortunately for our study of the nature up to now, most of our physical systems have avoided this problem, and the whole

quantum and statistical mechanics of non-dissipative systems can be given in terms of a Lagrangian or Hamiltonian formulation. Now, for dissipative systems there have been two main approaches. The first one consists of keeping the same Hamiltonian formalism for the whole system where the interacting background is included, as a result, one brings about a master equation with the dissipation and diffusion parameters appearing as part of the solution (Caldeira and Legget 1983, Unruh and Zurek 1989, and Hu et al 1992). This approach has its own merit, but it will not be followed in this paper. We will follow the second approach which consists in to obtain a phenomenological velocity depending Hamiltonian, representing a classical dissipative system, and to proceed to make the usual quantization (or statistical mechanics) with this Hamiltonian.

Within this last approach, one can, additionally, study the mathematical consistence of the the Hamiltonian formalism in quantum and statical mechanics. It is also known that even for one-dimensional systems, where the existence of their Lagrangian is guaranteed (Darboux 1894), the Lagrangian and Hamiltonian formulations are not free from problems (Havas 1973, Okubo 1980, Dodonov et al 1981, Marmon et al 1985, Glauber et al 1984, ^aLópez 1998, and ^bLópez 1999). One of the main problems is the implication on the quantization of the associated classical system when different Hamiltonians describe the same classical system (^cLópez 2002). This ambiguity has already been studied for the harmonic oscillator with dissipation and some general system (^dLópez 1996). In this paper, we want to show explicitly this ambiguity by studying the free falling particle within a medium which has the effect on the particle of producing the dissipation. This dissipation depends quadratically on the velocity of the particle. Firstly, two constants of motion are deduced for this system. Secondly, with these constants of motion two Lagrangian and two Hamiltonian are obtained using a known procedure (^dLópez 1996 and ^eLópez and Hernández 1989). Finally, using the Hamiltonian expression at first order in the dissipation parameter, the resulting eigenvalues of their associated quantum Hamiltonian and their associated statistical mechanics properties (for an ensemble of particles) are shown.

2 Constants of Motion

The motion of the particle of mass m falling under a constant gravitational force, $-mg$, where g is the constant acceleration due to gravity, which is within a dissipative medium which has the effect on the particle of producing a force proportional to the square of the velocity of the particle, $\alpha\dot{x}^2$ for $\dot{x} < 0$, can be described by the following autonomous dynamical system

$$\frac{dx}{dt} = v, \quad \frac{dv}{dt} = -g + \frac{\alpha}{m}v^2, \quad (1)$$

where the variable x represents the vertical position of the particle, and v represents its velocity. A constant of motion for this system is a function $K = K(x, v)$ such that $dK/dt = 0$, i.e. it satisfies the following equation (^fLópez 1999)

$$v \frac{\partial K}{\partial x} + \left(-g + \frac{\alpha}{m}v^2\right) \frac{\partial K}{\partial v} = 0. \quad (2)$$

The general solution of this equation is given by (John 1974)

$$K_\alpha(x, v) = G(C(x, v)), \quad (3)$$

where G is an arbitrary function of the characteristic curve $C(x, v)$. This characteristic curve can be given in two different ways as

$$C_1 = -\frac{mg}{2\alpha} \ln \left(1 - \frac{\alpha}{mg}v^2\right) + gx, \quad (4)$$

or

$$C_2 = \left(1 - \frac{\alpha}{mg}v^2\right) e^{-2\alpha x/m}. \quad (5)$$

Considering that one must obtain the usual constant of motion (Energy) expression for α equal to zero, the functionality of G in Eq. (3) is determined for each above characteristic ($G(C_1) = mC_1$ and $G(C_2) = -(mg/2\alpha)C_2 - m^2g/2\alpha$), and the following constants of motion are gotten

$$K_\alpha^{(1)}(x, v) = -\frac{m^2g}{2\alpha} \ln \left(1 - \frac{\alpha}{mg}v^2\right) + mgx, \quad (6)$$

and

$$K_\alpha^{(2)}(x, v) = \frac{m^2}{2\alpha} \left(-g + \frac{\alpha}{m}v^2\right) e^{-2\alpha x/m} + \frac{m^2g}{2\alpha}. \quad (7)$$

Note that the following limit is gotten

$$\lim_{\alpha \rightarrow 0} K_\alpha^{(i)} = \frac{1}{2}mv^2 + mgx \quad i = 1, 2. \quad (8)$$

3 Lagrangians and Hamiltonians

Using the know expression (Kobussen 1979, Leuber 1987, Yan 1981, and ^dLópez 1996),

$$L(x, v) = v \int \frac{K(x, v)}{v^2} dv , \quad (9)$$

to get the Lagrangian, the Lagrangian associated to Eq. (6) and Eq. (7) are

$$L_{\alpha}^{(1)}(x, v) = m\sqrt{\frac{mg}{\alpha}} v \operatorname{arc} \tanh \left(\sqrt{\frac{\alpha}{mg}} v \right) + \frac{m^2 g}{2\alpha} \ln \left(1 - \frac{\alpha}{mg} v^2 \right) - mgx \quad (10)$$

and

$$L_{\alpha}^{(2)}(x, v) = \frac{m^2}{2\alpha} \left(g + \frac{\alpha}{m} v^2 \right) e^{-2\alpha x/m} - \frac{m^2 g}{2\alpha} . \quad (11)$$

Their generalized linear momenta ($p = \partial L / \partial v$) are

$$p_{\alpha}^{(1)} = m\sqrt{\frac{mg}{\alpha}} \operatorname{arc} \tanh \left(\sqrt{\frac{\alpha}{mg}} v \right) \quad (12)$$

and

$$p_{\alpha}^{(2)} = mve^{-2\alpha x/m} . \quad (13)$$

Thus, their associated Hamiltonians, $H(x, p) = K(x, v(x, p))$, are given by

$$H_{\alpha}^{(1)}(x, p) = -\frac{m^2 g}{2\alpha} \ln \left[1 - \tanh^2 \left(\sqrt{\frac{\alpha}{mg}} \frac{p}{m} \right) \right] + mgx \quad (14)$$

and

$$H_{\alpha}^{(2)}(x, p) = \frac{m^2}{2\alpha} \left(-g + \frac{\alpha p^2}{m^3} e^{4\alpha x/m} \right) e^{-2\alpha x/m} + \frac{m^2 g}{2\alpha} , \quad (15)$$

where one has made the substitution of $p_{\alpha}^{(1)}$ and $p_{\alpha}^{(2)}$ by just p . One must note that the following limits are gotten

$$\lim_{\alpha \rightarrow 0} L_{\alpha}^{(i)}(x, v) = \frac{1}{2}mv^2 - mgx , \quad (16)$$

$$\lim_{\alpha \rightarrow 0} p_{\alpha}^{(i)} = mv , \quad (17)$$

and

$$\lim_{\alpha \rightarrow 0} H_{\alpha}^{(i)}(x, p) = \frac{p^2}{2m} + mgx \quad i = 1, 2 . \quad (18)$$

At first order in the dissipation parameter α , the Hamiltonians are given by

$$H^{(1)}(x, p) = \frac{p^2}{2m} + mgx - \frac{\alpha}{12m^4g}p^4 \quad (19)$$

and

$$H^{(2)}(x, p) = \frac{p^2}{2m} + mgx + \alpha \left(\frac{xp^2}{m^2} - gx^2 \right) . \quad (20)$$

4 Quantization at first order in perturbation theory

Our Hamiltonians Eq. (19) and Eq. (20) can be written as

$$H^{(i)}(x, p) = H_0(x, p) + W^{(i)}(x, p) \quad \text{for} \quad i = 1, 2 , \quad (21)$$

where H_0 represents the non dissipative part of the Hamiltonian,

$$H_0(x, p) = \frac{p^2}{2m} + mgx , \quad (22)$$

and $W^{(i)}$ represents the contribution of the dissipation at first order in α ,

$$W^{(1)}(x, p) = -\frac{\alpha p^4}{12gm^4} \quad (23)$$

and

$$W^{(2)}(x, p) = \alpha \left(\frac{xp^2}{m^2} - gx^2 \right) . \quad (24)$$

The Schrödinger equation, $i\hbar\partial\Psi(x, t)/\partial t = \hat{H}^{(i)}(\hat{x}, \hat{p})\Psi(x, t)$ represents an stationary problem. Therefore, in order to get the quantization of the system, one just need to solve the following eigenvalue problem

$$\hat{H}^{(i)}\Phi_n(x) = E_n^{(i)}\Phi_n(x) , \quad (25)$$

where $\hat{H}^{(i)}$ is the associated Hermitian operator of Eq. (21). Of course, one must not allow the particle to go beyond down the surface level. Thus, Eq. (22) is representing the Hamiltonian of the quantum bouncer ($x > 0$) (Gean-Banacloche 1999), where the eigenvalue problem

$$\hat{H}_0(\hat{x}, \hat{p})\psi_n^{(0)}(x) = E_n^{(0)}\psi_n^{(0)}(x) \quad (26)$$

has the eigenvectors and eigenvalues solution given by

$$\psi_n^{(0)}(x) = \frac{Ai(z - z_n)}{|Ai'(-z_n)|} \quad (27)$$

and

$$E_n^{(0)} = mgl_g z_n. \quad (28)$$

The functions Ai and Ai' are the Airy function and its differentiation respect to z . The variable z is defined as $z = x/l_g$, where l_g is given by $l_g = (\hbar^2/2m^2g)^{1/3}$, and z_n is the nth-zero of the Airy function ($Ai(-z_n) = 0$). In fact, the bouncing problem has already been studied for linear and quadratic dissipation (^gLópez 2004). For the later, the correction given to the eigenvalue problem using Eq. (24) at first order in perturbation theory is

$$\langle n|\hat{W}^{(2)}|n\rangle = \alpha \frac{4gl_g^2 z_n^2}{15}. \quad (29)$$

Now, using the relation $\langle n|d^4/dz^4|n\rangle = z_n^2/5$, the correction at first order in perturbation due to Eq. (23) is given by

$$\langle n|\hat{W}^{(1)}|n\rangle = -\alpha \frac{\hbar^4 z_n^2}{60gm^4 l_g^4}. \quad (30)$$

Therefore, for the same classical dynamical system we have two different associated quantum systems which have completely different quantum dynamics, which is shown through the eigenvalues

$$E_n^{(1)} = E_n^{(0)} + \alpha \frac{4gl_g^2 z_n^2}{15} \quad (31)$$

and

$$E_n^{(2)} = E_n^{(0)} - \alpha \frac{\hbar^4 z_n^2}{60gm^4 l_g^4}. \quad (32)$$

5 Classical Statistical model for dissipation

Consider a system of $N = N_1 + N_2$ particles, where N_1 particles are small of mass m_1 , and N_2 particles are big of mass m_2 ($m_2 \gg m_1$). The small particles move under the action of an external force with components $(0, 0, -mg)$ and suffer collisions with the walls of the container which consists in a narrow-square shape pipe of cross sectional area L^2 . In addition, each small particle can have occasional (stochastic) collision with the big particles, when they are added, establishes the dissipative medium where the big particles will move. The big particles move in this dissipative medium, and it is assumed that, since this type of collision does not occur frequently, its average effect may have neglected contribution on the dynamical macroscopic variables of the system. Newton's equations of motion for this system can be written as

$$m_1 \ddot{q}_{1ij} = 0 \quad j = 1, \dots, N_1; \ i = x, y \quad (33)$$

$$m_1 \ddot{q}_{1zj} = -m_1 g \quad j = 1, \dots, N_1 \quad (34)$$

$$m_2 \ddot{q}_{2ik} = \alpha (\dot{q}_{2ik})^2 \quad k = 1, \dots, N_2; \ i = x, y \quad (35)$$

$$m_2 \ddot{q}_{2zk} = \alpha (\dot{q}_{2zk})^2 - m_2 g \quad k = 1, \dots, N_2, \quad (36)$$

where q_{aij} , \dot{q}_{aij} and \ddot{q}_{aij} are the generalized coordinates, velocities and accelerations of the light-small ($a = 1$) and heavy-gross ($a = 2$) particles, and the parameter α characterizes the dissipative medium. The Hamiltonian associated the the motion of 1-particle, Eq. (33) and Eq. (34), is given by (^hLópez et al 1997)

$$H_{1;x,y,z} = \sum_{j=1}^{N_1} \left[\sum_{i=1}^3 \frac{p_{1ij}^2}{2m_1} + m_1 g q_{1zj} \right]. \quad (37)$$

The Hamiltonian associated to Eq. (35) is written as

$$H_{2;x,y} = \sum_{k=1}^{N_2} \sum_{i=1}^2 \frac{p_{2ik}^2}{2m_2} \exp \left(\frac{2\alpha q_{2ik}}{m_2} \right), \quad (38)$$

and, as we have seen in section 3, there are at least two Hamiltonians associated to Eq. (36) which are given by

$$H_{2;z}^{(1)} = \sum_{k=1}^{N_2} \left\{ -\frac{gm_2^2}{2\alpha} \ln \left[1 - \tanh^2 \left(\sqrt{\frac{\alpha}{m_2g}} \frac{p_{2zk}}{m_2} \right) \right] + m_2gq_{2zk} \right\} \quad (39)$$

and

$$H_{2;z}^{(2)} = \sum_{k=1}^{N_2} \left\{ \frac{p_{2zk}^2}{2m_2} \exp \left(\frac{2\alpha q_{2zk}}{m_2} \right) - \frac{m_2^2g}{2\alpha} \left[\exp \left(-\frac{2\alpha q_{2zk}}{m_2} \right) - 1 \right] \right\} . \quad (40)$$

Therefore, one has two different Hamiltonians to describe the same system, $H^{(1)} = H_{1;x,y,z} + H_{2;x,y} + H_{2;z}^{(2)}$ and $H^{(2)} = H_{1;x,y,z} + H_{2;x,y} + H_{2;z}^{(1)}$, which are written as

$$\begin{aligned} H^{(1)} = & \sum_{j=1}^{N_1} \left[\sum_{i=1}^3 \frac{p_{1ij}^2}{2m_1} + m_1gq_{1zj} \right] + \sum_{k=1}^{N_2} \sum_{i=1}^3 \frac{p_{2ik}^2}{2m_2} \exp \left(\frac{2\alpha q_{2ik}}{m_2} \right) \\ & + \sum_{k=1}^{N_2} \left\{ \frac{p_{2zk}^2}{2m_2} \exp \left(\frac{2\alpha q_{2zk}}{m_2} \right) - \frac{m_2^2g}{2\alpha} \left[\exp \left(-\frac{2\alpha q_{2zk}}{m_2} \right) - 1 \right] \right\} \end{aligned} \quad (41)$$

and

$$\begin{aligned}
H^{(2)} = & \sum_{j=1}^{N_1} \left[\sum_{i=1}^3 \frac{p_{1ij}^2}{2m_1} + m_1 g q_{1zj} \right] + \sum_{k=1}^{N_2} \sum_{i=1}^3 \frac{p_{2ik}^2}{2m_2} \exp \left(\frac{2\alpha q_{2ik}}{m_2} \right) \\
& + \sum_{k=1}^{N_2} \left\{ -\frac{gm_2^2}{2\alpha} \ln \left[1 - \tanh^2 \left(\sqrt{\frac{\alpha}{m_2 g}} \frac{p_{2zk}}{m_2} \right) \right] + m_2 g q_{2zk} \right\} .
\end{aligned} \tag{42}$$

Then, one can calculate for each Hamiltonian the canonical partition function (Toda et al 1998) which is associated to the same statistical system,

$$Z^{(i)} = \frac{1}{N_1! N_2! h^{3N}} \int \exp(-\beta H^{(i)}) dq dp \quad i = 1, 2 , \tag{43}$$

where β is defined as $\beta = 1/kT$ with k being the Boltzman's constant and T being the temperature, and the integration is carried out over all the coordinates and linear momenta of the two particles. The integration of momenta is carried out in the interval $(-\infty, +\infty)$. The integration on the transverse coordinates (x, y) is carried out in the interval $[0, L]$, and the integration of the vertical coordinate is carried out in the interval $[0, z]$. The partition functions for both cases are given by

$$\begin{aligned}
Z^{(1)} = & \frac{L^{2N_1}}{N_1! N_2! h^{3N}} \left(\frac{2\pi m_1}{\beta} \right)^{3N_1/2} \left(\frac{1 - e^{-\beta m_1 g z}}{\beta m_1 g} \right)^{N_1} \left(\frac{2\pi m_2}{\beta} \right)^{3N_2/2} \left(\frac{m_2}{\alpha} \right)^{2N_2} \times \\
& (e^{\frac{-\alpha L}{m_2}} - 1)^{2N_2} \left[\sqrt{\frac{\pi}{2\beta\alpha g}} e^{-\frac{\beta m_2^2 g}{2\alpha}} \left(\operatorname{Erfi} \left(\sqrt{\frac{\beta g m_2^2}{2\alpha}} e^{-\alpha z/m_2} \right) - \operatorname{Erfi} \left(\sqrt{\frac{\beta g m_2^2}{2\alpha}} \right) \right) \right]^{N_2}
\end{aligned} \tag{44}$$

and

$$\begin{aligned}
Z^{(2)} &= \frac{L^{2N_1}}{N_1!N_2!h^{3N}} \left(\frac{2\pi m_1}{\beta}\right)^{3N_1/2} \left(\frac{1-e^{-\beta m_1 g z}}{\beta m_1 g}\right)^{N_1} \left(\frac{2\pi m_2}{\beta}\right)^{N_2} \left(\frac{m_2}{\alpha}\right)^{2N_2} \\
&\quad \times (e^{-\frac{\alpha L}{m_2}} - 1)^{2N_2} \left(\frac{1-e^{-\beta m_2 g z}}{\beta m_2 g}\right)^{N_2} \left[\sqrt{\frac{\pi\alpha}{m_2^3 g}} \frac{\Gamma\left(\frac{\beta m_2^2 g}{2\alpha}\right)}{\Gamma\left(\frac{\beta m_2^2 g}{2\alpha} + \frac{1}{2}\right)} \right]^{N_2}.
\end{aligned} \tag{45}$$

The system has two internal energies, $U^{(i)} = -\partial \ln Z^{(i)} / \partial \beta$,

$$U^{(1)} = \left(\frac{5N_1}{2} + 2N_2\right) \frac{1}{\beta} - \frac{N_1 m_1 g z e^{-\beta m_1 g z}}{1 - e^{-\beta m_1 g z}} - \frac{N_2 m_2^2 g}{2\alpha} - \frac{N_2 f'(\beta)}{f(\beta)} \tag{46}$$

and

$$\begin{aligned}
U^{(2)} &= \left(\frac{5N_1}{2} + 2N_2\right) \frac{1}{\beta} - \frac{N_1 m_1 g z e^{-\beta m_1 g z}}{1 - e^{-\beta m_1 g z}} - \frac{N_2 m_2 g z e^{-\beta m_2 g z}}{1 - e^{-\beta m_2 g z}} \\
&\quad - \frac{N_2 m_2^2 g}{2\alpha} \left[\psi\left(\frac{\beta m_2^2 g}{2\alpha}\right) - \psi\left(\frac{\beta m_2^2 g}{2\alpha} + \frac{1}{2}\right) \right],
\end{aligned} \tag{47}$$

where the function $f(\beta)$ ($f'(\beta) = df(\beta)/d\beta$) has been defined as

$$f(\beta) = \operatorname{Erfi}\left(\sqrt{\frac{\beta g m_2^2}{2\alpha}} e^{-\alpha z/m_2}\right) - \operatorname{Erfi}\left(\sqrt{\frac{\beta g m_2^2}{2\alpha}}\right), \tag{48}$$

and $\operatorname{Erfi}(x) = -i\operatorname{Erf}(ix)$ is the complex error function which can be expressed in the form of the Dawson's integral, $\operatorname{Erfi}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2} \operatorname{Dawson}(x)$, $\operatorname{Dawson}(x) = e^{-x^2} \int_0^x e^{t^2} dt$ and ψ is the digamma function, $\psi(x) = d \ln \Gamma(x) / dx$. Thus, one can have two heat capacity expressions for the system, $C_V^{(i)} = \partial U^{(i)} / \partial T = -k\beta^2 \partial U^{(i)} / \partial \beta$,

$$C_V^{(1)} = \left(\frac{5N_1}{2} + 2N_2\right) k - \frac{N_1 k (m_1 g z \beta)^2 e^{-m_1 g z \beta}}{(1 - e^{-m_1 g z \beta})^2} + N_2 k \beta^2 \left(\frac{f''(\beta)}{f(\beta)} - \frac{(f'(\beta))^2}{(f(\beta))^2} \right) \tag{49}$$

and

$$C_V^{(2)} = \left(\frac{5N_1}{2} + 2N_2 \right) k - \frac{N_1 k (m_1 g z \beta)^2 e^{-m_1 g z \beta}}{(1 - e^{-m_1 g z \beta})^2} - \frac{N_2 k (m_2 g z \beta)^2 e^{-m_2 g z \beta}}{(1 - e^{-m_2 g z \beta})^2} + N_2 k \left(\frac{m_2^2 g \beta}{2\alpha} \right)^2 \left[\psi^{(1)} \left(\frac{m_2^2 g \beta}{2\alpha} \right) - \psi^{(1)} \left(\frac{m_2^2 g \beta}{2\alpha} + \frac{1}{2} \right) \right], \quad (50)$$

where $\psi^{(1)}$ is the trigamma function, $\psi^{(1)}(x) = d^2\Gamma(x)/dx^2$. Figure 1 shows the difference $|C_V^{(1)} - C_V^{(2)}|$ as a function of $\beta = 1/kT$. As one can see, this difference is not small at low temperatures (high β values). From β lower than about 2100, C_{V_2} is higher than C_{V_1} , and the situation is reversed for higher values. This difference seems to have an important implication related with the ergodic hypothesis (Toda et al 1998). Assuming the validity of the hypothesis, one would expect not difference at all on the calculated heat capacities (or internal energies) since averaging over the time variable must bring about the same value for both Hamiltonians (they represent the same dynamical system). However, averaging over the canonical ensemble must be different if the Hamiltonians are different. This ambiguity will remain when quantum canonical ensemble is considered (using Eq. (31) and Eq. (32)) for quantum statical analysis of the system.

6 Conclusions

We have shown two constants of motion, two Lagrangians, and two Hamiltonians for a free falling particle moving in a media with quadratic velocity dissipative force. These quantities describe the same dynamics of the classical system, but their quantization and the associated statistical mechanics (for an ensemble of particles) describe two different quantum and statistical dynamics. We have showed this at first order in the dissipative parameter and at first order in perturbation theory. There is still a point which remains to study and has to deal with quasi-classical limit. The question is whether or not both quantum Hamiltonians, Eq. (21), describes the same quasi-classical dynamics ($\hbar \rightarrow 0$) and coincides with the classical dynamics in this limit. We will deal with this problem and hope to report some results soon.

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Figure Captions

Difference of the heat capacities as a function of $\beta = 1/kT$ for $\alpha = 0.01$, $g = 1$, and $m_1/m_2 = 0.1$

